

Báez-Duarte's Criterion for the Riemann Hypothesis and Rice's Integrals

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Abstract

Criterion for the Riemann hypothesis found by Báez-Duarte involves certain real coefficients c_k defined as alternating binomial sums. These coefficients can be effectively investigated using Nörlund-Rice's integrals. Their behavior exhibits characteristic trend, due to trivial zeros of zeta, and fading oscillations, due to complex zeros. This method enables to calculate numerical values of c_k for large values of k , at least to $k = 4 \cdot 10^8$.

We give explicit expressions both for the trend and for the oscillations. The first tends to zero and is therefore, in view of the criterion, irrelevant for the Riemann hypothesis. The oscillations can be further decomposed into a series of harmonics with amplitudes diminishing quickly. Possible violation of the Riemann hypothesis would indicate that the amplitude of some high harmonic increases.

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1 Introduction

Several years ago a new expansion for the Riemann zeta function has been found by the author [6], [1]:

$$\zeta(s) = \frac{1}{s-1} \sum_{k=0}^{\infty} \frac{\Gamma(k+1-\frac{s}{2})}{\Gamma(1-\frac{s}{2})} \frac{A_k}{k!} \equiv \frac{1}{s-1} \sum_{k=0}^{\infty} \left(1-\frac{s}{2}\right)_k \frac{A_k}{k!} \quad (1)$$

where

$$A_k := \sum_{j=0}^k (-1)^j \binom{k}{j} (2j-1) \zeta(2j+2) \equiv \sum_{j=0}^k \binom{k}{j} \frac{\pi^{2j+2}}{(2)_j (\frac{1}{2})_j} B_{2j+2} \quad (2)$$

and

$$(x)_k \equiv \frac{\Gamma(k+x)}{\Gamma(x)}$$

is the Pochhammer symbol (having such an unfortunate denotation and sometimes called the rising factorial). Pochhammer symbols are in fact polynomials in variable x with integer coefficients equal to the Stirling numbers of the first kind. Since A_k tend to zero fast enough as $k \rightarrow \infty$ expansion (1) converges uniformly on the whole complex plane.

In fact, there exists a whole class of expansions similar to (1). The crucial thing is to remove the single pole of $\zeta(s)$ in $s=1$ which may be achieved either by multiplication by $s-1$ (or by any other function having single simple zero at unity) or by subtraction of $\frac{1}{s-1}$ (or by any other function having single simple pole at unity). In the second case we get a series converging even faster:

$$\zeta(s) = \frac{1}{s-1} + \sum_{k=0}^{\infty} \frac{\Gamma(k+1-\frac{s}{2})}{\Gamma(1-\frac{s}{2})} \frac{A_k}{k!} \quad (3)$$

where

$$A_k := \sum_{j=0}^k (-1)^j \binom{k}{j} \left(\zeta(2j+2) - \frac{1}{2j+1} \right) \quad (4)$$

One has also the freedom of choosing the "node" points at which expressions (1) or (3) give exact values, however the choice of even positive integers seems most natural, since A_k may be expressed by Bernoulli numbers and appropriate powers of π avoiding values such as $\zeta(3)$.

Finally, one can go all the way writing

$$\zeta(s) = \frac{1}{2(s-1)} \left[1 + s \left(\log(2\pi) - 1 + s \sum_{k=0}^{\infty} \frac{\Gamma(k+1-\frac{s}{2})}{\Gamma(1-\frac{s}{2})} \frac{A_k}{k!} \right) \right] \quad (5)$$

with

$$A_k := \sum_{j=0}^k (-1)^j \binom{k}{j} f(2j+2)$$

and

$$f(s) := \frac{\frac{2(s-1)\zeta(s)-1}{s} + 1 - \log(2\pi)}{s}$$

where $f(s)$ is also regular on the whole complex plane. One can check that expansion (5) gives exact values $\zeta(0) = -\frac{1}{2}$ as well as $\zeta'(0) = -\frac{1}{2} \log(2\pi)$ irrespective of how many terms in the series is taken into account.

In 2003 Luis Báez-Duarte, investigating expansion (1), found an interesting criterion for the Riemann hypothesis (RH) [2]. The crucial thing is to estimate the asymptotic behavior of certain real numbers defined as

$$c_k := \sum_{j=0}^k (-1)^j \binom{k}{j} \frac{1}{\zeta(2j+2)}. \quad (6)$$

More precisely, RH is equivalent to the statement that

$$c_k \ll k^{-3/4+\varepsilon}, \forall \varepsilon > 0. \quad (7)$$

If

$$c_k \ll k^{-3/4}$$

then all zeros of ζ are simple whereas regardless of the validity of the RH (unconditionally)

$$c_k \ll k^{-1/2}.$$

As Báez-Duarte pointed out, criteria of this type, i.e. relating RH to values of zeta at integer points, were known for a long time, however this one is definitely simpler and well-fitted for numerical investigations. Such investigations were performed numerically by the author in 2003 leading to the observation (which was surprising for us at that time) that the global behavior of coefficients c_k may be split into a trend (which dominates for low k not exceeding roughly 10^4) and subtle oscillations superimposed on this trend. (Similar splitting has been found by the author in the case of Li criterion for the RH, however in this case the oscillations are much more chaotic [7].)

2 Binomial transforms and asymptotics

Of course, such behavior may be well understood in the theory of binomial transforms using Rice's integrals (already known by Nörlund). Sums of this type can be interpreted as high order differences of appropriate numerical sequences $\{\varphi_k\}$. They were carefully investigated [4], see also [10]. The main result is (cf. Theorem 2 in [4]):

$$\sum_{k=n_0}^n (-1)^k \binom{n}{k} \varphi(k) = -(-1)^n \sum_s \operatorname{Res} \left[\varphi(s) \frac{n!}{s(s-1)\dots(s-n)} \right] \quad (8)$$

The proof of this fundamental theorem consists in applying classic Cauchy residue formula.

In the case of (6) we have $n_0 = 0$ and $\varphi(s) = 1/\zeta(2s+2)$, which is analytic on $[0, \infty[$ and meromorphic on the whole complex plane \mathbb{C} , therefore it fulfils the assumptions of the above theorem.

3 Results

It is clear that the problem is to find all poles of suitable function, in our case $1/\zeta(s)$. These poles are due to simple zeros of zeta in $s = -2n$ as well as due to complex zeros which we write as $\rho = \frac{1}{2} \pm i\gamma$. (Obviously if RH were true then all γ s would be real.) It is a matter of elementary exercise to find that for $n = 1, 2, \dots$ the residues in real poles are:

$$\operatorname{Res} \left(\frac{1}{\zeta(s)}; s = -2n \right) = \frac{1}{\zeta'(-2n)} = 2 \frac{(-1)^n (2\pi)^{2n}}{(2n)! \zeta(2n+1)} \quad (9)$$

where the last equality is a consequence of the functional equation for the zeta function.

Using main theorem (8) and (9) we find that the asymptotic form of the trend which stems from trivial zeros is

$$\begin{aligned} \bar{c}_k &= -\frac{k!}{\pi^{3/2}} \sum_{m=2}^{\infty} \frac{(-1)^m \pi^{2m}}{\Gamma(k+m+1) \Gamma(m - \frac{1}{2})} \frac{1}{\zeta(2m-1)} \\ &= -\frac{1}{4\pi^2} \sum_{m=2}^{\infty} \frac{B(k+1, m)}{\Gamma(2m-1)} \frac{(-1)^m (2\pi)^{2m}}{\zeta(2m-1)} \end{aligned} \quad (10)$$

(the latter being numerically still more effective) whereas the oscillating part due to complex zeros in the critical strip is:

$$\begin{aligned}\tilde{c}_k &= k! \sum_{\rho} \frac{\Gamma\left(\frac{1+\rho}{2}\right)}{\Gamma\left(k+1+\frac{1+\rho}{2}\right)} \operatorname{Res}\left(\frac{1}{\zeta(2s+2)}; s = -\frac{1+\rho}{2}\right) \\ &= \sum_{\rho} B\left(k+1, \frac{1+\rho}{2}\right) \operatorname{Res}\left(\frac{1}{\zeta(2s+2)}; s = -\frac{1+\rho}{2}\right)\end{aligned}\quad (11)$$

where $B(x, y)$ is the Euler beta function and $c_k = \bar{c}_k + \tilde{c}$. Both (10) and (11) converge quickly, hence they are suitable for numerical estimations contrary to the direct approach using the main definition (6) which becomes very time-consuming as k grows. What's more, values of zeta function at positive even integers should be calculated with many significant digits. Since $\zeta(2n)$ tends quickly to unity as n grows it is advisable, when using (6), to tabulate appropriate number of high-precision values of $\zeta(2n) - 1$ to preserve sufficient amount of significant digits as well as to avoid repeated unnecessary calculations. Nevertheless, calculating of the single coefficient c_{300000} took about 2 weeks on a fast cluster of four computers [12]. On the other hand, formulas (10) and (11) are much more effective: obtaining $c_{1000000}$ is a matter of few tens of seconds on a modest machine. In numerical calculations using (11) the function `NResidue` implemented in *Mathematica* proved especially useful. Figures 1–5 and the table below present the results.

k	c_k
10^5	$+1.60976 \cdot 10^{-9}$
$2 \cdot 10^5$	$-7.89739 \cdot 10^{-9}$
$3 \cdot 10^5$	$+5.82876 \cdot 10^{-9}$
$4 \cdot 10^5$	$-2.89364 \cdot 10^{-9}$
$5 \cdot 10^5$	$-3.45567 \cdot 10^{-9}$
$6 \cdot 10^5$	$+1.13652 \cdot 10^{-9}$
$7 \cdot 10^5$	$+3.14429 \cdot 10^{-9}$
$8 \cdot 10^5$	$+2.00526 \cdot 10^{-9}$
$9 \cdot 10^5$	$-1.70316 \cdot 10^{-10}$
10^6	$-1.77502 \cdot 10^{-9}$
$2 \cdot 10^6$	$+8.08716 \cdot 10^{-10}$
$3 \cdot 10^6$	$-8.22419 \cdot 10^{-10}$
$4 \cdot 10^6$	$+8.01923 \cdot 10^{-10}$
$5 \cdot 10^6$	$+2.78245 \cdot 10^{-10}$
$6 \cdot 10^6$	$-5.00102 \cdot 10^{-10}$
$7 \cdot 10^6$	$-5.21564 \cdot 10^{-10}$

The residues in (11) may be expressed by complex zeros of ζ in a manifest way. Introduce function $\xi(s) = \xi(1-s)$ as usual

$$\xi(s) := 2(s-1)\pi^{-s/2}\Gamma\left(1+\frac{s}{2}\right)\zeta(s).$$

Since ξ may be factorized using Hadamard product

$$\xi(s) = \prod_{\rho} \left(1 - \frac{s}{\rho}\right)$$

(the product being taken over paired complex zeros ρ) one can see that the residue of $1/\xi(s)$ in each particular pole ρ may be expressed as a function of all remaining ρ s. Let us label consecutive complex zeros as ρ_i according to the increase of $|\gamma|$. Choose further a particular zero ρ_n and introduce certain "crippled" function ξ_k as

$$\begin{aligned} \xi(s) &= (s - \rho_n) \xi_n(s) \\ \xi_n(s) &: = -\frac{1}{\rho_n} \left(1 - \frac{s}{\rho_n^*}\right) \prod_{i=1}^{n-1} \left(1 - \frac{s}{\rho_i}\right) \prod_{i=n+1}^{\infty} \left(1 - \frac{s}{\rho_i}\right) \end{aligned} \tag{12}$$

$1/\xi_k(s)$ is obviously regular at ρ_k and

$$\text{Res} \left(\frac{1}{\zeta(2s+2)}; s = -\frac{1+\rho_n}{2} \right) = -\frac{1}{2} \frac{h(\rho_n^*)}{\xi_n(\rho_n)} \quad (13)$$

where asterisk denotes complex conjugation and

$$h(s) := 2(s-1)\pi^{-s/2}\Gamma\left(1+\frac{s}{2}\right)$$

which is regular at ρ . Formula (13) is not very useful in practice since the product over paired complex zeros converges slowly, nevertheless, when combined with (11), gives an explicit formula relating any \tilde{c}_k to complex zeros ρ .

Using different approach Báez-Duarte gave another version of explicit formula of this kind, cf. [2], Theorem 1.5. The present approach is based entirely on Nörlund-Rice's integral and provides, I believe, immediate and more natural interpretation for the existence of oscillatory component of the coefficients c_k which is completely hidden in their primary definition (6). After all, the behavior of this very component is crucial for the RH, see Fig. 5. Last not least, resulting formulas are more handy and more effective in numerical calculations.

4 Discussion and open questions

Having any criterion for the RH the key thing is to say how "useful" it may be in numerical experiments. For example, Li's criterion states that RH is true if certain numbers λ_n are positive [7]. However, the fact that n initial λ_n are positive implies that roughly only \sqrt{n} complex zeros lay on the critical line [9]. Since high λ_n are extremely difficult to compute we can honestly say that Li's criterion, although very elegant, is pretty useless in practice. The natural question arises now: does the fact that k initial c_k obeys (7) implies that certain number m of initial complex zeros lay on the critical line? What is the relation between k and m ? Below we present simple argument based on formulas derived in this paper.

The consecutive residues (13) seem to be bounded sequence of complex numbers, cf. Fig. 6, so we neglect their influence. Using Euler beta function expansion for large values of its first argument [13]

$$B(a, b) \propto \Gamma(b)a^{-b} \left[1 - \frac{b(b-1)}{2a} \left(1 + O\left(\frac{1}{a}\right) \right) \right], \quad |a| \rightarrow \infty \quad (14)$$

we get:

$$B\left(k+1, \frac{1+\rho}{2}\right) \propto (k+1)^{-\frac{1+\rho}{2}} \Gamma\left(\frac{1+\rho}{2}\right) = \quad (15)$$

$$= \Gamma\left(\frac{1+\rho}{2}\right) (k+1)^{-\frac{3}{4}} \left[\cos\left(\frac{\gamma}{2} \log(k+1)\right) + i \sin\left(\frac{\gamma}{2} \log(k+1)\right) \right] \quad (16)$$

It is clear that if γ is real then we get bounded oscillations in \tilde{c}_k and, in the view of (7), RH is satisfied. Suppose, however, that there exists somewhere defiant extremely high zero $\frac{1}{2} + i\gamma$ with γ having non-vanishing imaginary part. (More precisely, there should be four such zeros at once placed symmetrically with respect to the critical axis and the real axis.) We are now sure that such a zero, if any, lies higher than $\gamma \simeq 10^{13}$ [5], [11] and probably higher than $\gamma \simeq 10^{21}$ [8]. This non-vanishing imaginary part would cause the trigonometric functions in (16) to acquire, roughly speaking, growing amplitudes thus violating criterion (7). Now, the amplitude of such growing oscillations would be extremely small due to elementary properties of the Euler beta function which appears in (11). Specifically, for $\gamma = 2 \cdot 10^{21}$ (which is not much higher than the range acquired recently by Odlyzko) the amplitude due to the corresponding zero is roughly $10^{-3.5 \cdot 10^{21}}$. Of course, the task to extract this particular harmonic, let alone to check whether its amplitude grows, is far beyond any numerical capabilities. In other words, even if the relatively low complex zero of zeta, say the hundredth, had some small shift off the critical line we would not be capable of finding this using (7) since its amplitude, in the sense of (16), is about 10^{78} times smaller than the amplitude of the first zero.

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This is rather sad news for all those who wish to (dis)prove the celebrated RH using simple criteria. On the other hand, estimations like that presented above enable one to understand why this problem is so tough. The Holy Grail and immortality it would bring to persistent searcher remain still out of reach... Well, perhaps there exists even simpler explanation to this mystery, explanation not involving all that terrible mathematics. *All things work together for good to them that love God* says the inscription on Bernhard Riemann's tomb taken from St. Paul's *Epistle to the Romans* (8:28). Shouldn't these words be taken for a clue? Yet, for a century and a half

many mathematicians would sell their souls for the proof. Clearly, there is an apparent contradiction between such a deal and St. Paul's words.

Figure captions

Fig. 1. Coefficients c_k for k up to 10^4 exhibit no apparent sign of oscillations. After calculating numerically the first 10^3 coefficients c_k this looked as "a pleasant smooth curve" [3].

Fig. 2. Million coefficients c_k computed using (10) and (11). Only 6 initial terms of the series were needed to accomplish sufficient accuracy.

Fig. 3. The same as Fig. 2 with logarithmic scale in k .

Fig. 4. Behavior of c_k (yellow) may be split into strictly growing trend (red) plus the oscillating part (blue) here plotted in the logarithmic k -scale. Initially the trend dominates over the oscillations but it tends to zero faster than these oscillations.

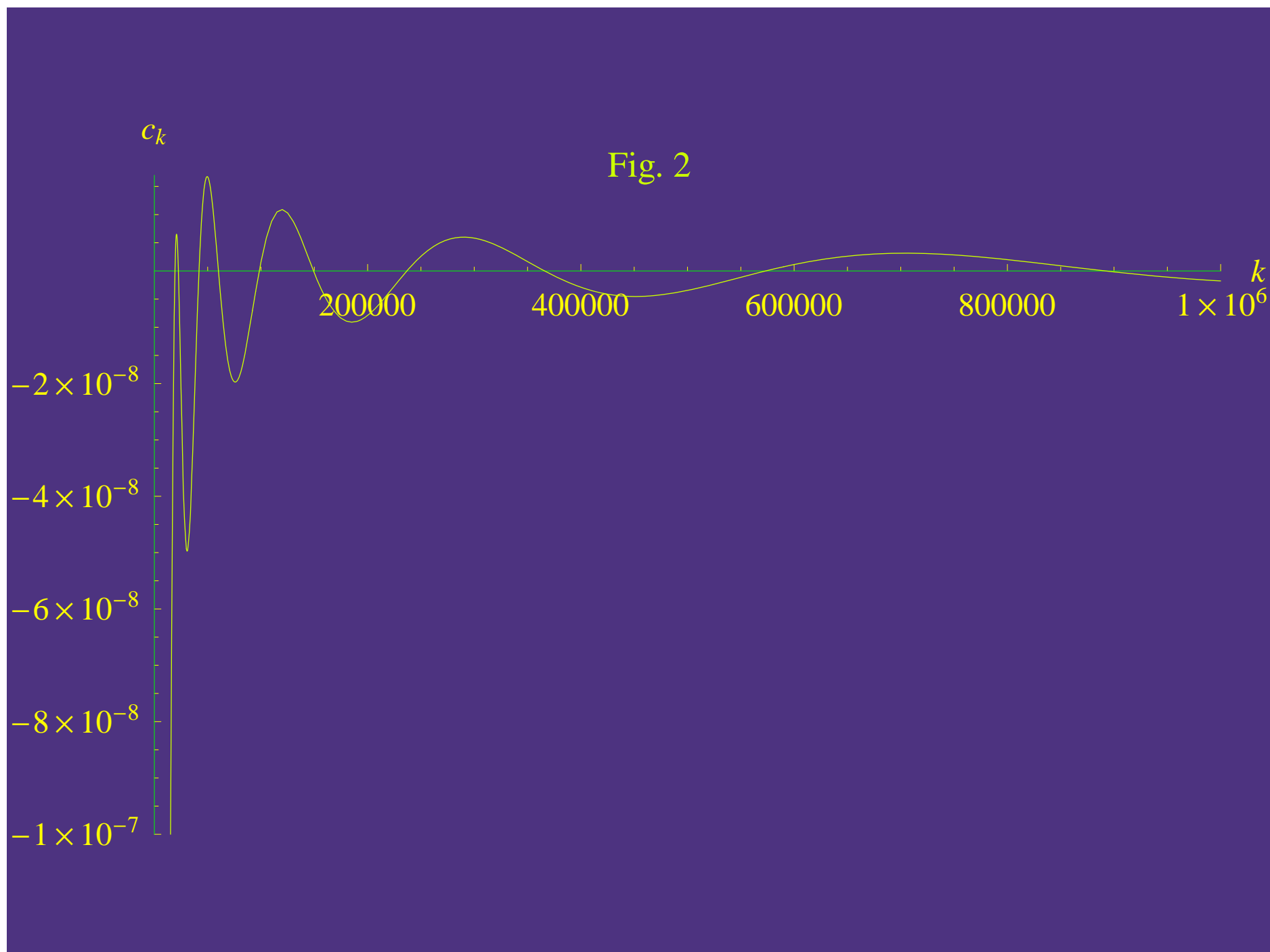
Fig. 5. Over 44 million components of c_k : trend \bar{c}_k (red) and oscillating part \tilde{c}_k (blue), both multiplied by $k^{3/4}$ (compare RH criterion (7)). The former grows strictly to zero whereas the latter seems to tend to perfect sine wave which is dominated by the first zero. (Amplitudes of further zeros diminish quickly.) If this tendency persisted to infinity *for all zeros* RH would be true. Maximum value of $k = 44700000$ is related to parameter `$MinNumber` in a particular version of *Mathematica*.

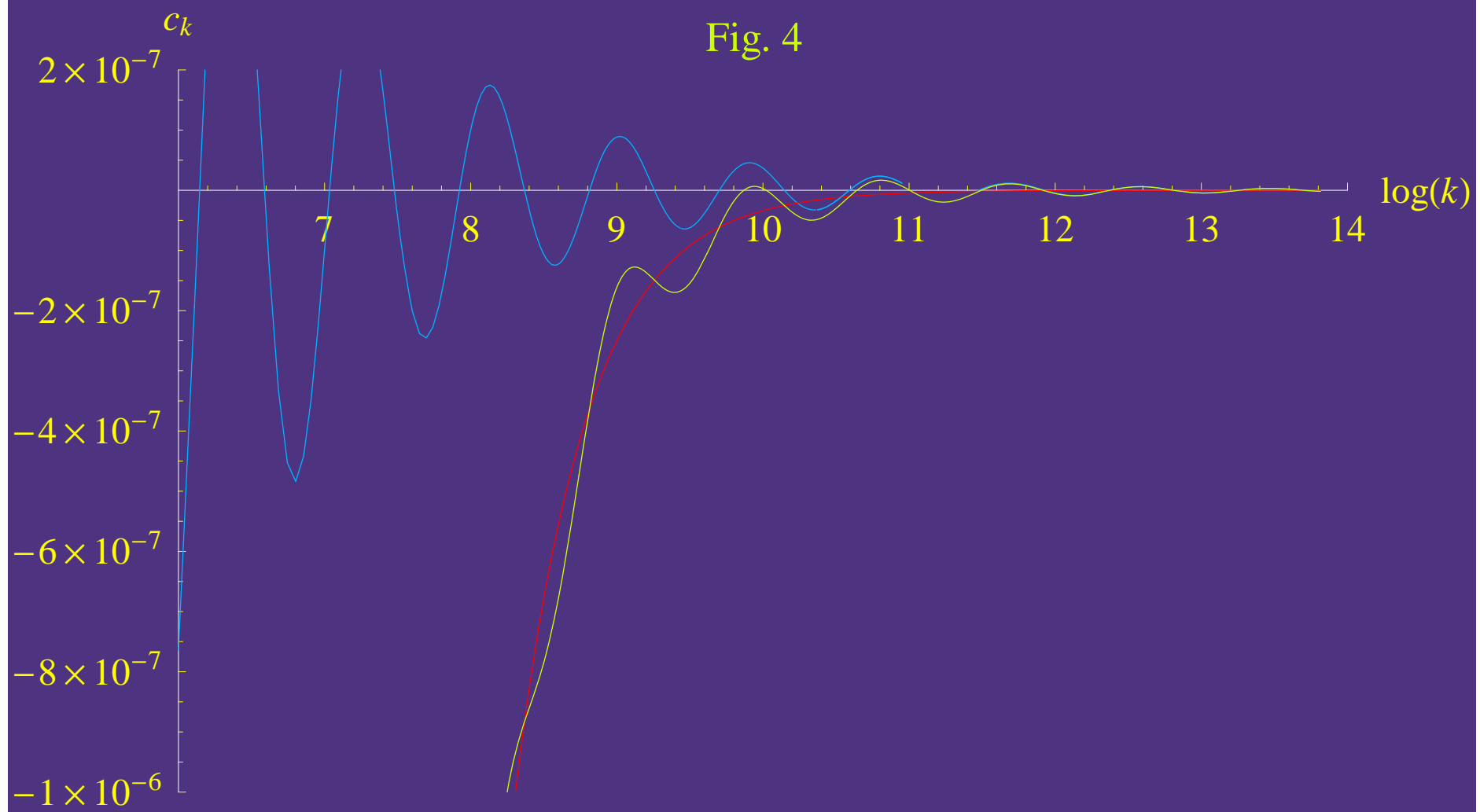
Fig. 6. 600 initial residues (13). Red color denotes real part, green – imaginary part. Points are joined together in order to better visualize their behavior.

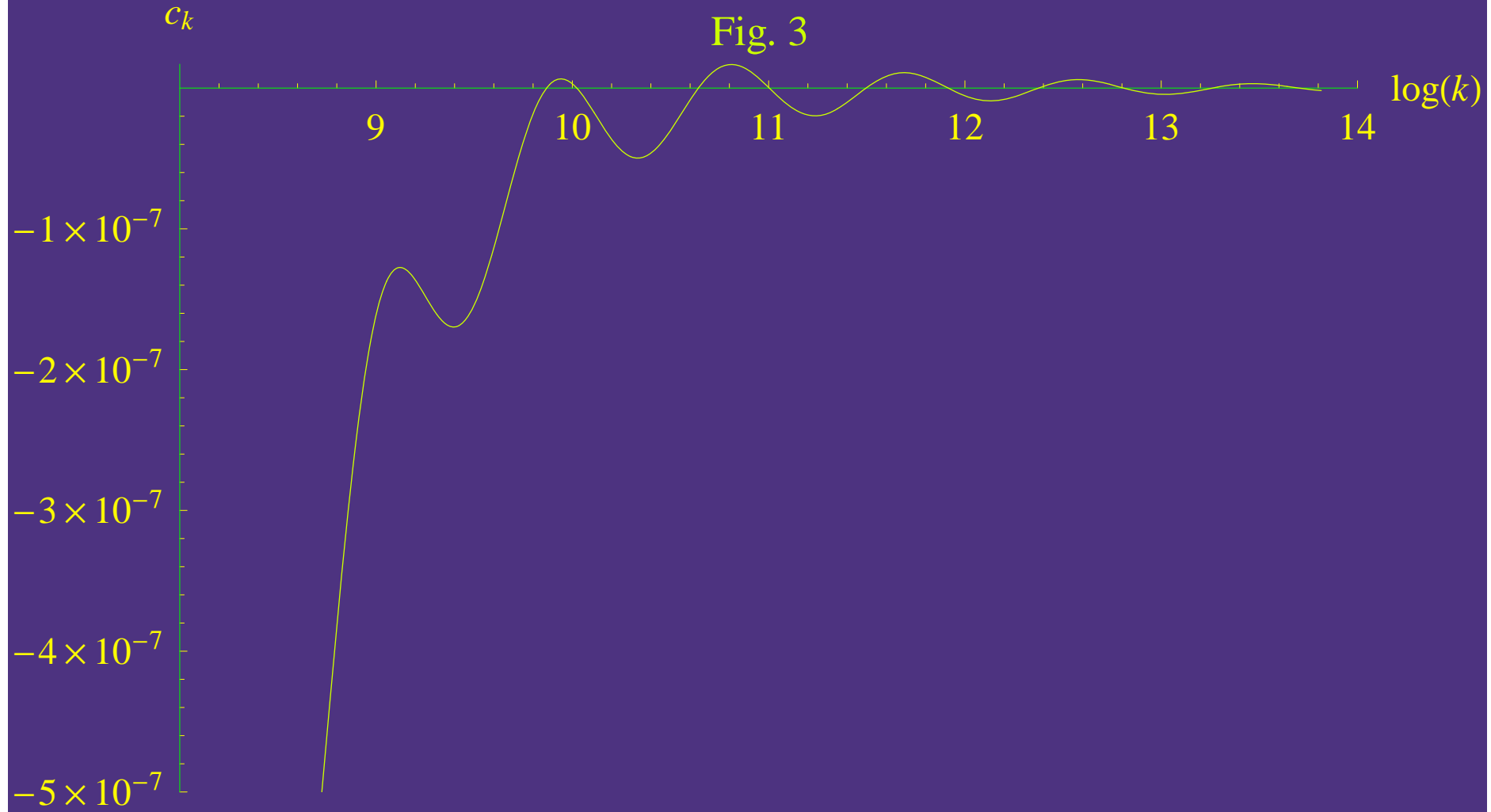
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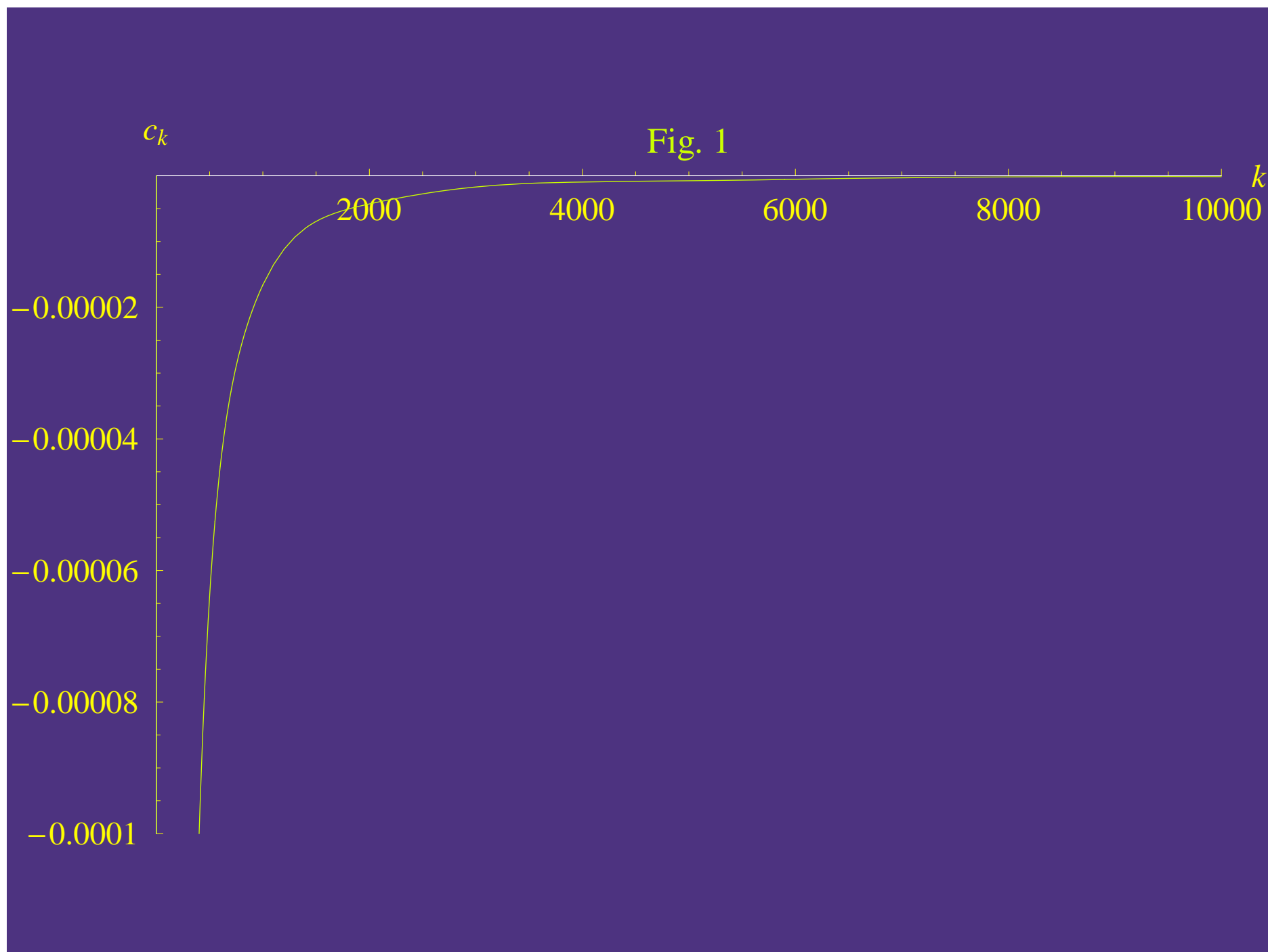


Fig. 5

